Structural characteristics of the protein hydration water

Franci Merzel[1,2] and Jeremy C. Smith[2]

[1] National Institute of Chemistry, Ljubljana, Slovenia
[2] Computational Molecular Biophysics, IWR, University of Heidelberg, Germany

Abstract

An understanding of the properties of protein hydration water is necessary for an understanding of protein folding, internal dynamics and function. Here, using molecular dynamics simulation, we provide an explanation of recent solution scattering data that indicate that the density of water on the surface of lysozyme is significantly higher than that of bulk water. The simulation-derived scattering profiles are in excellent agreement with experiment. In the simulation the 0.3nm-thick first hydration layer is 15% denser than bulk water. About two-thirds of this increase is due to a geometric contribution that would also be present if the water were unperturbed from the bulk. The remaining third arises from modification of the water structure and dynamics, involving approximately equal contributions from shortening of the water-water O...O distance and an increase in the coordination number. The first hydration shell density is shown to be correlated both with electrostatic properties of the protein surface and local surface topography as well as with the ordering of water molecules.